CONTENTS

LIST OF ABBREVIATIONS AND SYMBOLS

AO	Atomic Orbital
AOM	Angular Overlap Method
AP	Adiabatic Potential
CCA	Coupled Cluster Approach
CFT	Crystal Field Theory
CI	Configuration Interaction
CNDO	Complete Neglect of Differential OverlapP
DF	Dirac-Fock
DS	Dirac-Slater
DVM	Discrete Variation Method
DZ	Double Zeta
EHT	Extended Hückel Theory
HAO	Hybrid Atomic Orbital
GF	Green Function
GVB	Generalized Valence Bond
INDO	Intermediate Neglect of Differential Overlap
JTE	Jahn-Teller Effect
LCAO	Linear Combination of Atomic Orbitals
LFT	Ligand Field Theory
LHP	Longuet-Higgins-Pople
LMO	Localized Molecular Orbital
MBPT	Many-Body Perturbation Theory
MC SCF	Multiconfiguration Self-Consistent Field
MM	Molecular Mechanics
MO	Molecular Orbital
NDDO	Neglect of Diatomic Differential Overlap
PCILO	Perturbative Configuration Interaction using Localized Orbitals
PF	Primitive Function
PT	Perturbation Theory
PZ	Poly Zeta
REX	Relativistic Extended Hückel
RHF	Restricted Hartree-Fock
SCF	Self-Consistent Field
SCP	Slater-Condon Parameter
SOI	Spin-Orbit Interaction
STO	Slater-Type Orbital
SZ	Single Zeta
UHF	Unrestricted Hartree-Fock
VB	Valence Bond
ZDO	Zero Differential Overlap

a^*	complex conjugate of a
$\underline{a}$	vector a
$\hat{A}$	operator of the physical quantity A
$\bar{A}$, $\langle A \rangle$	mean value of the physical quantity A
$\mathbf{A}$	vector potential of electromagnetic field
$\mathbf{A}$	matrix with elements A_{ij}
$\mathbf{A}^{-1}$	inverse matrix to A
$\mathbf{A}^T$	transposed matrix to A, $(A^T)_{ij} = A_{ji}$
$\mathbf{A}^+$	hermitian conjugate to A, $(A^+)_{ij} = A^*_{ji}$
$\|a\rangle$	ket vector
$\langle a\|$	bra vector
$\{a\}$	column matrix (vector)
$\{a\}^T$	row matrix (vector)
$\hat{A}_n$	antisymmetrization operator of n particles
A_i^A	electron affinity of i-th orbital of atom A
$a \times b$	vector product of the vectors a and b
$a.b$	scalar product of the vectors a and b
$[\hat{A},\hat{B}]_-$	commutator of the operators $\hat{A}$ and $\hat{B}$
$[\hat{A},\hat{B}]_+$	anticommutator of the operators $\hat{A}$ and $\hat{B}$
$\mathbf{B}$	magnetic field induction
c	speed of light in vacuum
$\mathbf{C}$, $\mathbf{C}^\alpha$, $\mathbf{C}^\beta$	matrix of LCAO coefficients
$\mathbf{d}$	dipole moment vector
$det(\mathbf{A})$	determinant of the matrix A
e	elementary charge
$E_i(R)$	adiabatic potential
E_i^{el}	electronic energy
$\mathbf{F}$	force constant matrix
$\hat{F}$	Fock operator
g	electronic g-factor
g_N	nuclear g-factor
$\hat{g}(1,2)$, $\hat{g}$	two-electron operator
$\mathbf{G}$	electron interaction matrix
$G_{kl}(\omega)$	Fourier transform of the one-electron Green function
$G_{pq,rs}$	supermatrix of electron repulsion integrals
h	Planck constant
$\hbar$	reduced Planck constant ($\hbar = h/2\pi$)
$\hat{h}(1)$	one-electron operator
$\hat{h}^{so}$	operator of the spin-orbit interaction

i	imaginary unit
$\mathbf{I}$	unit matrix with the elements δ_{ij}
I_N	angular momentum of a nucleus
I_i^A	ionization energy of i-th orbital of atom A
$(ik\|jl)$	two-electron integral of electron repulsion
$\langle ij\|g\|kl\rangle$	two-electron integral of electron repulsion
$\mathbf{j}$	total angular momentum of electron
$\hat{J}_l$	Coulomb operator
J_{ij}	Coulomb integral over spinorbitals
$\hat{K}_l$	exchange operator
K_{ij}	exchange integral over spinorbitals
k	Boltzman constant
$\mathbf{l}$	orbital angular momentum of electron
m_A	mass of A-th nucleus
m_e	mass of electron
m_0	rest mass of a particle
n	number of electrons
N	number of atoms in a molecule
N_A	Avogadro constant
occ	occupied molecular (spin) orbital
$\hat{P}$	projection operator
$\mathbf{P}$, $\mathbf{P}^\alpha$, $\mathbf{P}^\beta$	charge density (bond-order) matrix
p_i	linear momentum of a particle
$\hat{P}_n$	spin-free n-particle density function
$\hat{Q}$	operator complementary to $\hat{P}$
R	gas constant
$\mathbf{s}$	spin angular momentum of electron
S_{ij}	overlap integral
T	temperature
T_{ij}	kinetic integral
$Tr(\mathbf{A})$	trace of the matrix $\mathbf{A}$
$\mathbf{U}$	matrix of a unitary transformation
V_A^C	averaged integral of electron-nuclear attraction
$V_{i_A j_B}^C$	integral of electron-nuclear attraction
vir	unoccupied (virtual) molecular (spin) orbital
X_i^A	Mulliken orbital electronegativity
$\hat{X}_j$	annihilation operator
$\hat{X}_i^+$	creation operator
Z_A	proton number of A-th nucleus
Z_A^c	core charge in units of e

α	spin-up function ($m_s = +1/2$)
β	spin-down function ($m_s = -1/2$)
β	Bohr magneton
β_N	nuclear magneton
$\hat{\gamma}_n$	Dirac operators (matrices of dimension 4 x 4)
γ_{AB}	averaged integral of electron repulsion
Γ_a	representation of a symmetry point group
$\Gamma_a \otimes \Gamma_b$	direct product of representations
δ_{ij}	Kronecker symbol
$\delta(r)$	Dirac function
$\Delta = 10Dq$	parameter of the ligand-field strength
ϵ_0	vacuum permittivity
ϵ_i	orbital energy
$\sum'_{i,j}$	summation omitting the terms with i = j
$\eta_k(s_k)$	spin function
ζ	orbital exponent
$\vartheta_k(r_k)$	atomic orbital
λ	wavelength
$\bar{\mu}$	magnetic moment vector
ν	frequency of radiation
$\tilde{\nu}$	wavenumber
$\xi(r_i)$	constant of the spin-orbit interaction
$\rho(r)$	charge density
σ_{SI}	conversion factor to SI units ($\sigma_{SI} = e^2/4\pi\epsilon_0$)
$\hat{\underline{\sigma}}$	vector of Pauli matrices ($\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$)
$\hat{\sigma}_n$	Pauli matrix of dimension 2 x 2
$\varphi_k(r_k)$	molecular orbital
Φ	electrostatic potential
Φ_u	determinantal wave function (Slater determinant) of the electron configuration
Φ_i^a	wave function of the monoexcited configuration
Φ_{ij}^{ab}	wave function of the biexcited configuration
χ_k	primitive basis set function
$\psi_k(x_k)$	spinorbital
Ψ	wave (state) function
∇	vector operator 'nabla'